Syllabus

CHEM 558- Nanocrystals: Fundamentals of Inorganic Materials at the Nanoscale

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Overview: This course is designed for graduate students and senior undergraduates to provide a detailed investigation into the chemical and physical principles underlying inorganic nanocrystals.

Lectures: Tues. & Thurs., 10:50 AM – 12:05 PM, George R. Brown Hall West, Room 212

Textbooks and Reading: There are no required texts for this course. All relevant reading material will be provided throughout the semester as a pdf available in Canvas. The course material is primarily taken from the following texts:

- Rohrer, G. S. *Structure and Bonding in Crystalline Materials*. Cambridge University Press: 2001
- Woodward, P. M.; Karen, P.; Evans, J. S. O.; Vogt, T. *Solid State Materials Chemistry*. Cambridge University Press: 2021
- Somorjai, G. A. *Introduction to Surface Chemistry and Catalysis*. Wiley-VCH: 2010
- Callister, W. D. *Materials Science and Engineering: An Introduction*. Wiley-VCH: 2013
- Shriver, D.; Atkins, P.; *Inorganic Chemistry*. W.H. Freeman: 2009
- Young, R. J.; Lovell, P. A.; *Introduction to Polymers*. CRC Press: 2011
- Israelachvili, J. N. *Intermolecular and Surface Forces*. Elsevier: 2011
- Hiemenz, P. C.; Rajagopalan, R. *Principles of Colloid and Surface Chemistry*. CRC Press: 1997
- Kittel, C. *Introduction to Solid State Physics*. Wiley-VCH: 2004

Grading: Learning and comprehension will be evaluated via four major components: homework, literature reviews, a final proposal project, and participation.

Homework (30%)- Designed to solidify key principles by working through problems. Students are welcome to work together on homework assignments but each individual must turn in their own work.

Literature Reviews (30%)- Recent papers from the literature will be assigned for reading. Students will provide a written report following the guideline provided below, due the morning of literature review days (see course schedule). The class session will then consist of an open discussion of the motivations, data, conclusions, and future potential of the manuscript. Participation in literature review classroom sessions is mandatory.

Proposal Project (30%)- Students will propose a novel research project, designed to investigate a new concept or technology involving nanocrystals. Evaluation will be based on a written proposal and an oral presentation. Emphasis will be on novelty, scientific feasibility, and clarity of communication.

Participation (10%)- Evaluation will be based on attendance in class, discussion during lecture, and participation in literature review sessions.

Office Hours: By appointment only. Email Prof. Jones for scheduling.

Academic Integrity: Students are expected to adhere to the Rice University Code of Student Conduct and uphold the Honor System with respect to cheating and plagiarism. This material is available in the Student Handbook or online at the following web address: http://students.rice.edu/students/Student_Handbook1.asp.

Disability Resources: If you have a documented disability that may affect academic performance, you should: 1) make sure this documentation is on file with Disability Support Services (Allen Center, Room 111 / adarice@rice.edu / x5841) to determine the accommodations you need; and 2) meet with Prof. Jones to discuss your accommodation needs.

General Expectations: Treat your peers and your instructor with respect. Work hard and put in the time to understand the material. Ask frequent questions. Contact Prof. Jones *immediately* with any concerns, scheduling conflicts, or confusion about the course material. Problems are *always* easier to address and mitigate when discovered early.

Course Summary: The field of inorganic nanocrystals is one of the most well-developed in all of nanoscience. In fact, the birth of experimental nanotechnology can be traced back to several key experiments involving the observation of size-dependent properties in semiconductor nanocrystals. Because quantum mechanical and surface-based effects can completely dominate the behavior of the system, these materials display some of the most striking examples of size-dependent phenomena. In addition, nanocrystals are playing an increasingly important role in next generation optics, energy storage, and biomedical technologies. Therefore, a deep fundamental understanding of the chemical and physical principles that drive the formation, stabilization, size-dependent properties, and assembly of these materials is necessary from both a fundamental and application-driven perspective. However, because nanocrystals exist at a size scale that is intermediate between molecules and bulk materials, most coursework treats this material tangentially and views the subject as either a scaled-up version of chemistry or a scaled-down version of materials science. In this course we will focus exclusively on the topic of inorganic nanoscale structures and, as a result, we will take an integrated approach to understanding the field. Concepts from chemistry, physics, chemical engineering, and materials science will all be important for establishing a complete understanding of this unique class of matter. Students will benefit from a focused and interdisciplinary approach to learning this subject.

Learning Objectives: After completing the course students will have a strong grasp for the physical chemical principles governing the major aspects of inorganic nanocrystal science. This will cover a range of topics including but not limited to: nucleation and growth, crystal faceting, surface ligand chemistry, size-dependent properties and scaling relationships, interparticle forces, nanoparticle self-assembly, and major characterization tools. A strong emphasis will be placed on understanding how an inorganic nanocrystal-based system will respond to an external stimulus and how these responses are different from their bulk counterparts. This will develop a strong connection between fundamental concepts and practical observations that will benefit students in laboratory research. Regular discussion of topical literature will create familiarity with the most exciting and impactful research in the field and allow for critical evaluation of experimental science. Finally, a proposal project at the end of the course will require a deeper dive into a specific area, provide experience with grant writing, and foster creativity in project design.

Course Schedule (topics and timing are subject to change)

Unit 1: Structure and Synthesis		
Week 1	11-Jan	Introduction to Nanocrystals
	13-Jan	Crystallography- Bravais lattices, points, directions, planes
Week 2	18-Jan	Surfaces- facets, energetics, reconstructions, epitaxy
	20-Jan	Crystal defects- volumetric, planar, linear, point
		Written Literature Review 1 Due
Week 3	25-Jan	Nucleation and Growth (I)- supersaturation, critical radius, LaMer model
	27-Jan	Nucleation and Growth (II)- seeded syntheses, heterogeneous nucleation, growth modes
		Homework 1 Due
Week 4	1-Feb	Particle Shape (I)- equilibrium and surface considerations
	3-Feb	Particle Shape (II)- kinetic and defect considerations
		Written Literature Review 2 Due
Unit 2: Surface ligands, Particle Interactions, Assemblies		
Week 5	8-Feb	Adsorption Equilibria- Langmuir model and modifications thereof
	10-Feb	Spring Recess - No Class
		Homework 2 Due
Week 6	15-Feb	Polymeric Ligands- persistence length, conformation, confinement, polymer brush
	17-Feb	Small Molecule Ligands- SAMs, size-dependent packing
		Written Literature Review 3 Due
Week 7	22-Feb	Organometallic Bonding- covalent, X-type, L-type, Z-type
	24-Feb	Interparticle Interactions (I)- pair potentials, thermal energy, soft matter, sterics
		Homework 3 Due
Week 8	1-Mar	Interparticle Interactions (II)- Van der Waals, electrostatic, depletion
	3-Mar	Interparticle Interactions (III)- multivalency and cooperativity
		Written Literature Review 4 Due
Week 9	8-Mar	Particle Assembly (I)- clusters
	10-Mar	Particle Assembly (II)- supercrystals and superlattices
		Homework 4 Due
Week 10	15-Mar	Spring Break - No Class
	17-Mar	Spring Break - No Class

Unit 3: Size-Dependent Properties		
Week 11	22-Mar	Plasmons (I)- conduction band oscillations, dielectric constant, resonant modes
	24-Mar	Plasmons (II)- coupling and hybridization, electric field concentration
		Written Literature Review 5 Due
Week 12	29-Mar	Plasmons (III)- applications, SERS, imaging, metamaterials
	31-Mar	Mechanics- elastic and plastic deformation mechanisms, scaling relationships
		Homework 6 Due
Week 13	5-Apr	Excitons (I)- band structure, particle in a box, dimensionality and density of states
	7-Apr	Excitons (II)- band alignment in core-shell particles, fermi's golden rule, lifetime
		Written Literature Review 6 Due
Week 14	12-Apr	Excitons (III)- applications, solar, displays, photocatalysis
	14-Apr	Buffer Class
Week 15	19-Apr	Oral Proposal Presentations
	21-Apr	Oral Proposal Presentations
Finals Week		No Final Exam

Written Literature Review Rubric: manuscript reports will be modeled on the peer review requirements of the American Chemical Society. Use the outline below to prepare your reports.

Rate the article in the following areas (Low, Medium, High, Highest- top 5%)
Significance:
Novelty:
Broad Interest:
Scholarly Presentation:

Answer the following questions about the manuscript (Yes, No, In Part)
Are the conclusions adequately supported by the data?
Are the literature references appropriate and correct?
Do the contents justify the length of the manuscript?

Summary of article

Assessment of potential impact on the scientific field, or impact on society in general (i.e. is it likely to influence or generate new research, or change the way we live). Note: additional readings may be required to understand the background and fully answer this question.

Areas of improvement- what needs to be changed about the paper, or what things are missing. If nothing, then list experiments that would have been interesting but not necessary.

Statement of future research- what should the next steps be? If the paper is fundamental, these should be basic scientific questions, along with planned experiments (in broad strokes, not an actual experimental plan). If the paper is highly applied, these should be the necessary steps to actually implement the material or technique in a real-world setting. Note: this will likely require additional research be convincing.

Reports should be 1-2 pages in length using the above formatting as a guide.

Grading will be based on:

1. Completeness and accuracy of description, including context of research
2. Critical evaluation of the techniques, data, interpretation, and conclusions
3. Creativity in follow-up plans
4. Adherence to the document format (e.g. includes all sections, correct length)

Literature reports are due on the day of the in-class literature discussion (see calendar). You may either turn in a printed copy or email a copy to mrj@rice.edu. Reports are due before or at the beginning of class.

Final Research Proposal Rubric: The proposed research can be related to any of the subject areas covered in the course. A topic must be submitted by the date provided in the syllabus to Prof. Jones for approval. It will take the form of a 200-300 word abstract with 1-5 references that states: a) the problem, challenge, or fundamental question to be examined; b) the basic strategy for conducting the research; c) the potential impact of achieving the research goal.

The research proposal will consist of an oral presentation and a written report; written reports are due the day of the oral presentation, TBD.

Oral Presentation: A professional powerpoint presentation will be given to the class providing the same basic information as the written document (see below). All students are expected to provide comments and questions to evaluate the work proposed by their peers. Presenters will be cut off if they go longer than 15 min. Because students will be evaluated on their ability to respond to comments, it is *highly recommended* that students target an uninterrupted presentation length of 10-12 min in order to leave time for questions.

Written Report: The document should be written in the style of a standard research proposal, aimed at obtaining funding for 1-2 full-time researchers for a 2-3 year period. Use of current research topics is not allowed. Topics *related* to a student's current research are allowed but must be sufficiently different and novel to warrant approval. All topics must be approved by Prof. Jones. Questions regarding the format or construction of the research proposal should be addressed as early as possible.

Specific guidelines and the format for the written document are given below:

> Brief Synopsis/Overview (<300 words)- A brief description of the overall project, written in simple, non-scientific terms. This can be the abstract you submitted previously.
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> Statement of Problem/Challenge (<300 words)- Identify a current problem or fundamental lack of knowledge in an area that is related to nanocrystalline materials, or that could potentially be solved via the application of inorganic nanocrystals.
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> Specific Aims/Goals (<150 words, should include at least three specific tasks/challenges)- A breakdown of the individual components of the research goal (e.g. materials to be made, properties to be measured, devices to be fabricated).
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> Background/Significance (2-5 pages)- The background information should include all relevant information on: The proposed problem, prior/current solutions and their limitations, all necessary materials and their synthetic/processing considerations, and all required experimental techniques.
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> Research Design and Methods (~5-8 pages)- This section needs to break down the specific aims introduced earlier, developing a series of experiments to achieve each goal. The methodology should be clearly documented, along with sufficient information to explain and justify the experimental approach. This section should also address potential challenges and pitfalls, as well as strategies to alter the experimental plan to address these, should they arise. Finally, although experiments do not need to be performed, hypothesized results should be proposed based on an understanding of the scientific literature and topics presented in the course lectures.
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> Future Research (<300 words)- Proposed plans for follow-up work based on the results and conclusions from the initial experiments. What new experiments, understanding, and/or applications are enabled by the proposed work?

Grading will be based on:

1. Novelty of the proposed work and potential impact on the field
2. Feasibility of the project and use of appropriate experimental methods
3. Clarity of communication in both written and oral presentation formats
4. Adherence to the document format (e.g. includes all sections, correct length)